

Isopentyl lactate
19329-89-6 | DTXSID00858801

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.98e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.29e-01

Confidence level: 5.71e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Naphthylamine</div> <div>Measured: 4.00e-01</div> <div>Predicted: 9.37e-04</div>	<div>Image not found</div> <div>2-Butanone, 1-bromo-</div> <div>Measured: 1.26e-01</div> <div>Predicted: 7.89</div>	<div>Image not found</div> <div>Ethyl isobutyrate</div> <div>Measured: 3.75</div> <div>Predicted: 19.3</div>
<div>Image not found</div> <div>Phenyl phosphorodichloridate</div> <div>Measured: 5.23e-02</div> <div>Predicted: 1.16e-02</div>	<div>Image not found</div> <div>Nonylamine</div> <div>Measured: 1.55e-01</div> <div>Predicted: 2.75e-01</div>	